DTU Civil Engineering
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DANISH TECHNOLOGICAL INSTITUTE

CONCRETE EXPERTCENTRE

Mass transport and chemical modeling

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Outline

- Status of the project
- Chemical module
  - Implementation in this project
  - Extension to other models
- Coupled water and moisture transport
  - General formulation
  - Hysteresis modeling
  - Test examples
- Future work
- Conclusion

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Status of project

- Implementation status of 1D finite element code

TRANSPORT PROCESSES

Mass transport modeling will include:

- Diffusion of ions ✓
- Electromigration ✓
- Vapor/liquid transport ✓
- Sorption hysteresis ✓
- Diffusion of gasses

CHEMICAL EQUILIBRIUM

Chemical module for establishing of equlibrium

- Solid solution models ✓
- Surface complexation models
- Detailed cement paste model
- Chemical boundary model

COUPLED MODEL ✓

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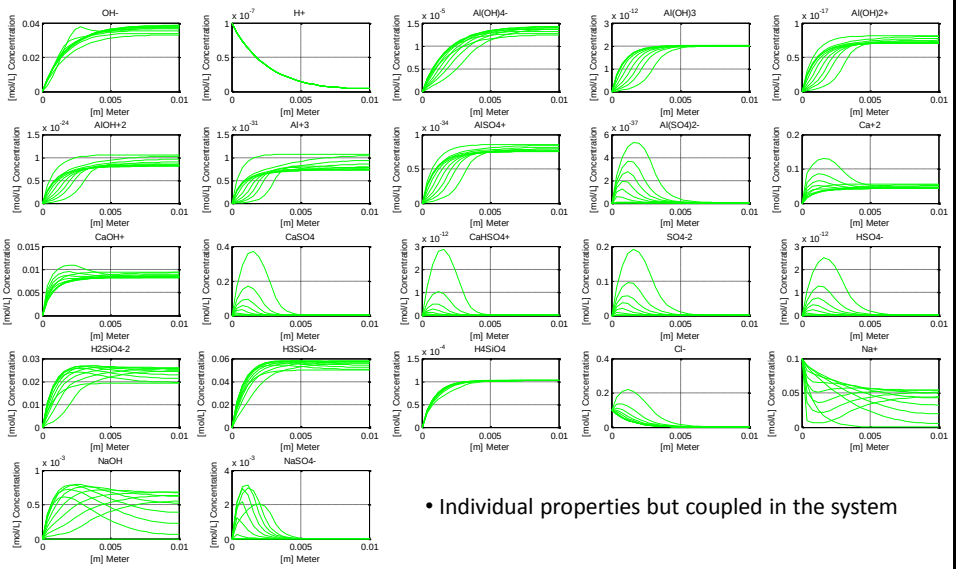
Status of project (summary)

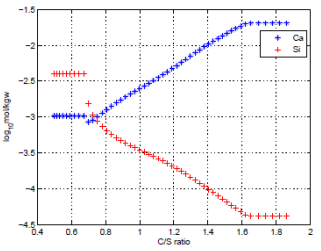


- Individual properties but coupled in the system

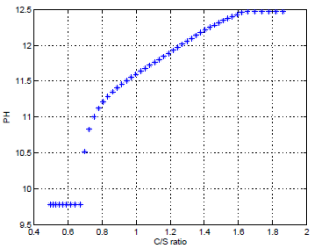
Status of project (summary)

CSH model – with focus on C/S ratio and PH development

$$(CaO)_{0.66}(SiO_2)(H_2O)_{1.5} + 1.32H^+ \leftrightarrow 0.66Ca^{2+} + H_4SiO_4 + 0.16H_2O$$
$$(CaO)_{0.83}(SiO_2)_{0.66}(H_2O)_{1.83} + 1.66H^+ \leftrightarrow 0.83Ca^{2+} + 0.66H_4SiO_4 + 1.34H_2O$$
$$(CaO)_{1.33}(SiO_2)(H_2O)_{2.16} + 2.66H^+ \leftrightarrow 1.33Ca^{2+} + H_4SiO_4 + 1.49H_2O$$
$$(CaO)_{1.5}(SiO_2)_{0.66}(H_2O)_{2.5} + 3.00H^+ \leftrightarrow 1.50Ca^{2+} + 0.66H_4SiO_4 + 2.68H_2O$$
$$Ca(OH)_2 + 2H^- \leftrightarrow Ca^{2+} + 2H_2O$$
$$SiO_2 + 2H_2O \leftrightarrow H_4SiO_4$$



(a) Total Ca and Si concentration in solution with respect to Ca/Si in solid solution



(b) PH in pore solution

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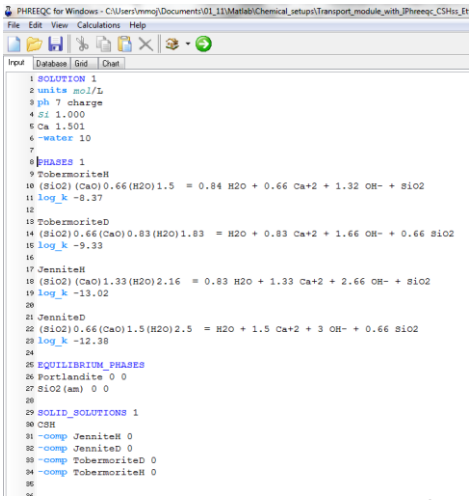
Chemical module

- General chemical module based on PHREECH
  - How does it work
- Solid – Liquid
  - Solid degradation
  - PH change
- Liquid – Gas
  - Carbonation

Remember that it is coupled to a mass transport, to evaluate the different models in a detailed manner.



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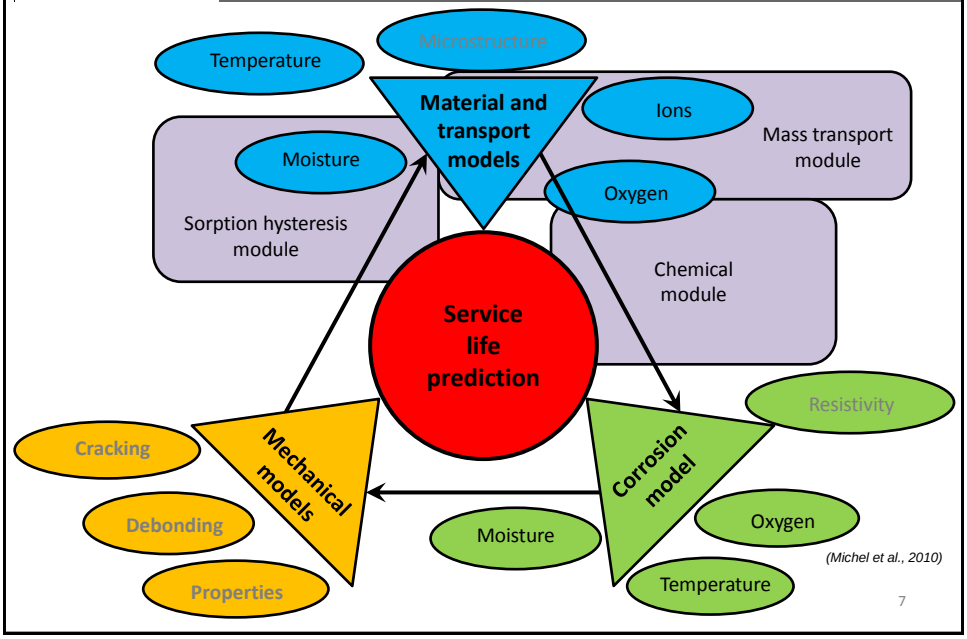
Chemical module



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Coupled water and moisture transport

- Governing equation
  - Diffusion of water

$$\rho_w \frac{\partial \varepsilon^l}{\partial t} = \nabla \cdot \left(D_{\varepsilon^l} \nabla \varepsilon^l \right) + r \left(\varepsilon^{l,eq} - \varepsilon^l \right)$$

  - Diffusion of moisture

$$\rho_{vs} \left(\varepsilon_p - \varepsilon^l \right) \frac{\partial \phi_v}{\partial t} - \rho_{vs} \phi_v \frac{\partial \varepsilon^l}{\partial t} = \nabla \cdot \left(D_\phi \nabla \phi_v \right) - r \left(\varepsilon^{l,eq} - \varepsilon^l \right)$$

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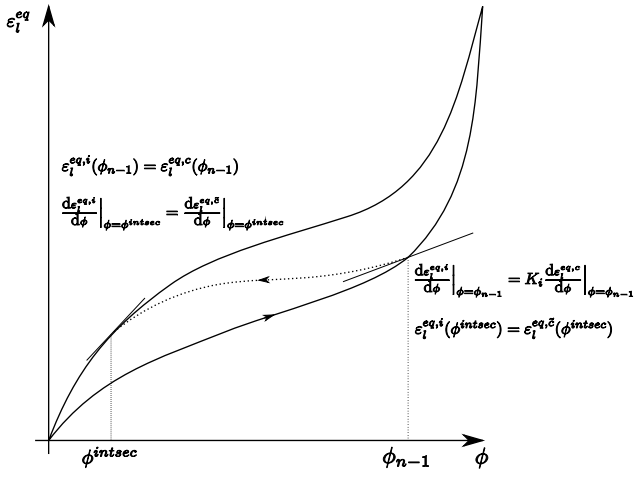
Coupled water and moisture transport

- 3 order polynomial sorption hysteresis
  - Generic example



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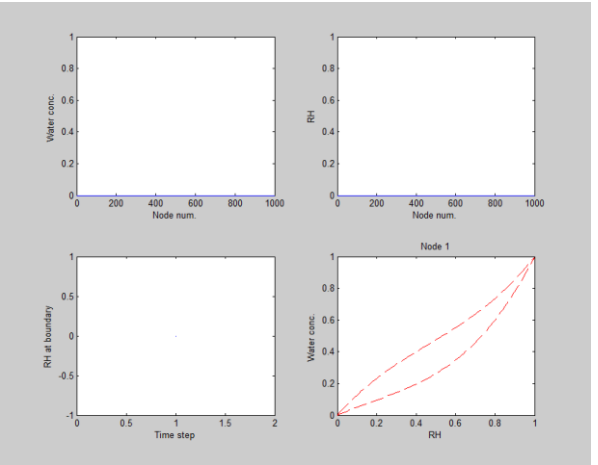
Coupled water and moisture transport

- Generic test example with time depended boundary conditions



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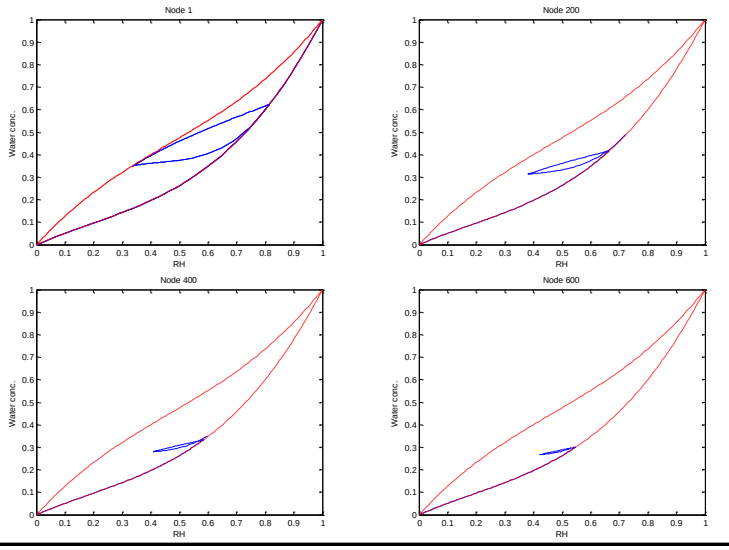
Coupled water and moisture transport

- RH and liquid concentration in 4 different nodes



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Future work

- Higher order polynomial for sorption isotherms
- Ensure numerical stability for coupled model
  - The individual parts are stable, but the coupled model require attention
- Assemble more detailed chemical models through literature study

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Conclusion

- Beta version of coupled model
  - Simulations of simple problems
  - Test of different chemical models
- Sorption hysteresis model
  - Tide variations and other similar variations